Continuous phase transition from Néel state to Z_2 spin-liquid state on a square lattice

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Abstract

Recent numerical studies of the J_1-J_2 model on a square lattice suggest a possible continuous phase transition between the Néel state and a gapped spin-liquid state with Z_2 topological order. We show that such a phase transition can be realized through two steps: First bring the Néel state to the U(1) deconfined quantum critical point, which has been studied in the context of Néel – valence bond solid (VBS) state phase transition. Then condense the spinon pair – skyrmion/antiskyrmion bound state, which carries both gauge charge and flux of the U(1) gauge field emerging at the deconfined quantum critical point. We also propose a Schwinger boson projective wave function to realize such a Z_2 spin liquid state and find that it has a relatively low variational energy($-0.4893J_1$/site) for the J_1-J_2 model at $J_2 = 0.5J_1$. The spin liquid state we obtain breaks the fourfold rotational symmetry of the square lattice and therefore is a nematic spin liquid state. This direct continuous phase transition from the Néel state to a spin liquid state may be realized in the J_1-J_2 model, or the anisotropic J_{1x}-J_{1y}-J_2 model.

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A spin liquid state has been searched for both theoretically and experimentally for decades, especially for the purpose of understanding the novel mechanism of high-T_c cuprates[1]. One of the most interesting and relevant models is the J_1-J_2 spin-1/2 antiferromagnetic Heisenberg model on a square lattice, since the frustration induced by the J_2 term in the J_1-J_2 model might mimic the frustration induced by the hopping term in the t-J model, which has been believed to be the low-energy effective model of high-T_c cuprates[2]. According to Anderson's resonating valence bond (RVB) scenario[3], the potential spin liquid state in the J_1-J_2 model might be the most important low-energy metastable state of cuprates and the superconducting ground state will be naturally developed upon doping[4]. On the other hand, the J_1-J_2 model can be realized in many frustrated magnets[5,6]; thus investigating the phase diagram of such a simple model would be of great importance by itself. Previous theoretical studies using the mean-field theory have found a possible Z_2 spin liquid phase in the J_1-J_2 model[7–9]. Very recently, a spin liquid ground state has been observed in the maximal frustrated region($J_2 \sim 0.5J_1$) by numerical studies[10,11]. The discovered spin liquid ground state has gaps in both spin singlet and triplet channels, and a universal constant $\gamma \simeq \ln 2$ in the entanglement entropy. These signatures indicate a gapped spin liquid with Z_2 topological order. Moreover, the numerical studies also show evidences for a continuous phase transition between the Néel state with antiferromagnetic ordering at the wave vector (π, π), and the (possible) Z_2 spin liquid state.

Studies of quantum phase transitions between quantum spin liquid phases and adjacent phases are important for the understanding of the spin liquid states, as they provide vital information on the effective field theory description of the spin liquid and also predict universal behaviors that can be compared with experimental and numerical results. However, in the past there has been no theory that can describe a continuous phase transition between the Néel state and a Z_2 spin liquid state in a model with the SU(2) spin rotational symmetry. Particularly, the theory of deconfined quantum criticality indicates that killing the antiferromagnetic order in the Néel state does not result in a symmetric paramagnetic state but a valence bond solid (VBS) state[12,13]. On the other hand, starting from a bosonic Z_2 spin liquid state, one can bring it to an antiferromagnetic state through a continuous phase transition by condensing the spinon excitations, but the resulting antiferromagnetic state has a noncollinear order[14,15], rather than the collinear order that the Néel state has. It is not until the work by Moon and Xu[16] that a continuous phase transition between a Z_2

spion liquid and a collinear antiferromagnetic state is proposed. In their theory they show that condensing bound states of spinon and vison excitations in the Z_2 spin liquid state leads to a continuous phase transition to a collinear antiferromagnetic state. However, their study is based on a field theory analysis and it is not clear what kind of specific SU(2) symmetric lattice model can support such a field theory.

In this work, we study the continuous phase transition between the Néel and the Z_2 spin liquid state on square lattice starting from the Néel state. We propose that the critical point of this phase transition is described by the same deconfined quantum critical theory that is also applicable to the critical point between the Néel and the VBS order. As a motivation, we consider a J_1-J_2-Q model that contains both next-nearest-neighbor interaction temrs and plaquette ring-exchange terms with coefficient Q. When $Q = 0$, this model is reduced to the J_1-J_2 model which has a phase transition from the Néel to the Z_2 spin liquid phase. When $J_2 = 0$, the J-Q model has been studied by the quantum Monte Carlo method[17] and it realizes the continuous phase transition from Néel to VBS phase described by the deconfined quantum critical theory. Based on these two limits we can conjecture a possible phase diagram of the J_1-J_2-Q model, as illustrated in Fig. 1, assuming that there are no other phases between the two limits and all phase transitions are of second order. In the phase diagram the phase boundaries between the Néel and the VBS state and between the VBS and the Z_2 spin liquid state[13] are both described by the theory of deconfined quantum criticality. As these two phase boundaries are connected to the phase boundary separating the Néel and the spin liquid state, it is likely that the latter is also described by the same deconfined quantum critical point. We note that a numerical study on the J_1-J_2-J_3 model[18] gives evidence for a similar phase diagram that contains the Néel phase, a plaquette VBS phase and possiblely a Z_2 spin liquid phase.

Moreover, we propose that the Z_2 spin liquid state is obtained from the deconfined quantum critical point by condensing the spinon pair–skyrmion/antiskyrmion bound state. In the theory of deconfined quantum criticality, the effective theory of the critical point is a CP(1) model that contains a spin-$\frac{1}{2}$ spinon field coupling to an emergent U(1) gauge field. Starting from this deconfined quantum critical point, one can gap out the spin excitations by proliferating topological defects known as the skyrmion and drive the system into the VBS state. On the other hand, one can also obtain a Z_2 spin liquid state by condensing a pair of spinon excitations, which acts as a Higgs field carrying gauge charge $2e$ of the emergent U(1)

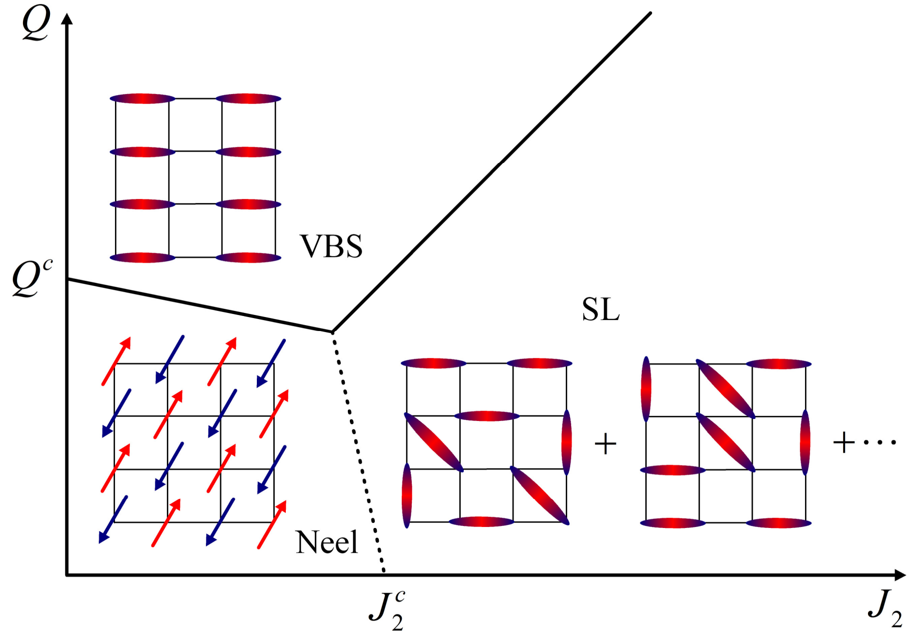


FIG. 1. Conjectured phase diagram of the J_1-J_2-Q model. In the phase diagram we set $J_1 = 1$ and vary the other two frustration terms. At the origin $J_2 = Q = 0$ the model is in the Néel state. Along the x axis $Q = 0$ and the model reduces to the J_1-J_2 model, which has a continuous phase transition between Néel and Z_2 spin liquid states[10,11]. Along the y axis $J_2 = 0$ and the model reduces to the J-Q model, which has a continuous phase transition between Néel and VBS order[17]. The solid lines show phase boundaries described by the deconfined quantum criticality[12,13], and the dashed line shows the phase boundary that is the subject of this study, in which we propose that it can also be described by the deconfined quantum criticality.

gauge field[14]. To achieve these two goals simultaneously, we propose a scenario where a Z_2 spin liquid state can be obtained from the deconfined quantum critical point by condensing the the spinon pair–skyrmion/antiskyrmion bound state.

One interesting feature of the Z_2 spin liquid state obtained in our study is that it breaks the four-fold rotational symmetry of the square lattice, or in other words it is a nematic spin liquid. This result is obtained by a symmetry analysis in Section I, and it is consistent with previous mean field studies[7–9]. Therefore we predict that on the square lattice if a gapped Z_2 spin liquid state is separated from the Néel state by a continuous phase transition, the spin liquid state should be nematic. We would like to emphasize that our theoretical study is generic and is not tied to any particular model Hamiltonian, though numerical evidences strongly suggest that it is very likely to be realized in the J_1-J_2 model and the anisotropic J_{1x}-J_{1y}-J_2 model. A detailed discussion will be presented in Section IV and V.

The rest of the paper is organized as the following: In Section I we discuss the scenario of a continuous phase transition from the Néel state to the Z_2 spin liquid state through bound-state condensation. We first briefly review the spinon and skyrmion/antiskyrmion excitations at the deconfined quantum critical point, and then discuss the scenario of obtaining a Z_2 spin liquid state from the deconfined quantum critical point by condensing the bound state of a spinon pair and a skyrmion/antiskyrmion. By studying the projective symmetry group (PSG) properties of the bound-state operators we identify the symmetry of the Z_2 spin liquid state. It turns out that the obtained Z_2 spin liquid state preserves all lattice symmetries except the fourfold rotational symmetry of the square lattice, and it is therefore a nematic spin liquid state.

In Sec. II we study the phase transition to the Z_2 spin liquid phase and the excitations in the spin liquid phase. We argue that a spin liquid phase can be obtained from the U(1) deconfined quantum critical point by proliferating spinon pair–skyrmion/antiskyrmion bound states. We also find two types of low-energy excitations in the Z_2 spin liquid state: spinons carrying spin-$\frac{1}{2}$ and visons that are vortex excitations of the bound-state condensate. In our theory both the spinon gap and vison gap close at the critical point, which is consistent with the numerical studies[10,11].

In Sec. III we construct a projective wave function for the Z_2 spin liquid state that we obtain by condensing the bound-state operator. The Schwinger boson projective wave function is a well-established way to describe the Néel state and adjacent spin liquid states[19,20], and it has been used to study the J_1-J_2 model on a square lattice[9,21]. Near the Néel state there are several different Schwinger boson projective wave functions describing Z_2 spin liquid states with different topological orders, and they can be classified using their PSG[22,23]. By matching the PSG of the projective wave function to the PSG of the bound-state operator in the effective theory, we are able to identify the particular Schwinger boson projective wave function that represents the Z_2 spin liquid state to which the Néel state can be connected through a continuous phase transition.

In Sec. IV we study the Schwinger boson projective wave function using the variational Monte Carlo method. Our calculation is based on the nonorthogonal valence bond basis[24], where the sign problem is manageable if the state is close to the U(1) deconfined quantum critical point. We show that this bosonic spin liquid state has a relatively low ground-state energy, and it can be stabilized by an anisotropy in the nearest-neighbor Heisenberg coupling $J_{1x} \neq J_{1y}$.

I. BOUND STATE OF SPINON-PAIR AND SKYRMION.

The starting point of our work is the theory of the deconfined quantum criticality introduced by Senthil *et al* in Ref. 12 and 13. Its main result is that the critical point between the Néel state and the VBS state is described by a non-compact CP(1) model that contains deconfined spin-$\frac{1}{2}$ spinon fields coupled to an emergent non-compact U(1) gauge field. The CP(1) model has the following Lagrangian,

$$\mathcal{L} = \frac{1}{g} \sum_{\alpha=\uparrow\downarrow} |(\partial_\mu - i a_\mu) z_\alpha|^2, \tag{1}$$

where z_α is a bosonic spinon field carrying spin-$\frac{1}{2}$ and it is related to the Néel order parameter $\boldsymbol{n} \sim (-1)^i \boldsymbol{S}_i$ in the following way,

$$\boldsymbol{n} = z_\alpha^* \boldsymbol{\sigma}_{\alpha\beta} z_\beta. \tag{2}$$

The gauge field a_μ in Eq. (1) is an emergent U(1) gauge field.

Another important part in the deconfined quantum criticality is the topological excitation in the Néel state, called the skyrmion. Skyrmion excitations are characterized by the skyrmion number Q, a topological invariant of the spatial configuration of the Néel order parameter $\boldsymbol{n}$, defined as the following,

$$Q = \frac{1}{4\pi} \int d^2x \boldsymbol{n} \cdot \partial_x \boldsymbol{n} \times \partial_y \boldsymbol{n}. \tag{3}$$

The physical meaning of Q is the total number of skyrmion excitations, and it is conserved for smooth space-time configurations of $\boldsymbol{n}$. However, in a lattice model, singular configurations of $\boldsymbol{n}$ with tunneling events between configurations with different skyrmion numbers are allowed. Therefore, in an effective theory, one needs to add by hand skyrmion creation and annihilation events. In the CP(1) model, skyrmion excitations are related to the gauge flux of a_μ because of the following relation,

$$2\pi Q = \int d^2x (\partial_x a_y - \partial_y a_x). \tag{4}$$

Hence we can relate skyrmion excitations to 2π flux quanta of the a_μ gauge field. The existence of skyrmion tunneling events is then equivalent to the existence of monopole events in the space-time configuration of the gauge field, or to the fact that the gauge field is compact.

The key result of the deconfined quantum criticality theory is that the skyrmion creation and annihilation events are irrelevant at the critical point, or in other words, the emergent U(1) gauge field is non-compact. The reason behind this is the non-trivial Berry phase associated with the skyrmion tunneling events[25], which takes four different values on four sublattices of the dual lattice. Because of this spatially dependent Berry phase, contributions of skyrmion tunneling events cancel each other unless the skyrmion number is changed by a multiple of four. As a result, skyrmion tunneling events become irrelevant at the critical point. Another consequence of this spatially dependent Berry phase is that the proliferation of skyrmion excitations leads to the breaking of lattice translational and rotational symmetry, and brings the system to the VBS state. This effect can be understood by considering the symmetry transformation of the skyrmion creation operator. The Berry phase associated to skyrmion tunneling events results in a non-trivial phase acquired by the skyrmion operator v after lattice symmetry transformations[13], as summarized in Table I. As a result, v can be related to the following linear combination of the order parameters of columnar VBS states since they have the same symmetry transformations[13]

$$v = e^{i\frac{\pi}{4}}(v_x + iv_y), \tag{5}$$

where v_x and v_y denote the order parameters for columnar VBS states in the x and y direction respectively. Hence the condensation of v leads to lattice symmetry breaking and therefore a VBS order.

Next, we discuss the scenario of obtaining a Z_2 spin liquid state from the deconfined quantum critical point through condensing a bound state of a skyrmion/antiskyrmion and a spinon pair. Starting from the deconfined quantum critical point, which has an emergent U(1) gauge field, a generic way of obtaining a Z_2 state is to condense a Higgs field that carries gauge charge $2e$[14]. On the other hand, in order to kill the Néel order, we will need to condense the skyrmion field. Consequently, we consider condensing a bound state of these two excitations, which can be expressed as a product of the two operators.

In the CP(1) model, a natural candidate of a charge-$2e$ Higgs field is a pair of spinons.

Since we are trying to get a spin liquid state, the Higgs field must be a spin singlet. Hence the field must contain at least one spatial derivative[14]. The possible forms at the lowest order are,

$$u_i = \epsilon_{\alpha\beta} z_\alpha \partial_i z_\beta, i = x, y. \tag{6}$$

Now we can write a bound-state operator as a product of skyrmion/antiskyrmion and spinon pair operators in Eq. (5) and (6). Actually there are more than one way to combine a skyrmion/antiskyrmion and a pair of spinons, as both the skyrmion/antiskyrmion and spinon pair fields have different components. This can be resolved by analyzing how the bound-state operator transforms under lattice symmetry operations. Since the Z_2 spin liquid state is obtained by condensing the bound-state operator, its symmetry transformations determine the symmetry of the spin liquid state. In order to obtain a spin liquid state with all lattice symmetries, we search for a bound-state operator that is invariant under lattice symmetry transformations.

One complication in the symmetry analysis of the bound-state operator is that because of the gauge charge it carries, it can carry a projective representation of the symmetry group[22], and therefore does not need to be in the trivial representation to be invariant under a symmetry operation. Particularly, the skyrmion operator acquires a non-trivial phase under the translation and condensing the skyrmion breaks the translational symmetry[13]. However, although the bound-state operator acquires the same phase under translation, such a phase can be canceled by a U(1) gauge transformation and the spin liquid state can still be translational invariant. Consequently, by condensing a bound state instead of the skyrmion alone, the translational symmetry is restored and a spin liquid state instead of the VBS state is obtained. As an example, consider the v_x component of the skyrmion operator v, as defined in Eq. (5), which acquires a minus sign upon translation in the x direction,

$$T_x : v_x \to -v_x, \tag{7}$$

and such symmetry transformation results in the translational symmetry breaking of the VBS states obtained by condensing v_x. On the other hand, the product of u_i and v_x carries gauge charge $2e$, and the minus sign that appears in Eq. (7) can be canceled by a gauge transformation of $z_\alpha \to i z_\alpha$. Therefore the state obtained by condensing $u_i v_x$ does not break the translational symmetry.

Because of the gauge covariance of the bound-state operator, we need to study its PSG property to fully understand the symmetries it has. The symmetry transformations of the CP(1) field, the skyrmion, and spinon pair operators are summarized in Table I. A summary of symmetry transformations of the CP(1) field can be found in Ref. 26, and the symmetry transformations of skyrmion operators are explained in Ref. 13.

	T_x	T_y	$R_{\pi/2}$	I_x	$\mathcal{T}$
z_α	$\epsilon_{\alpha\beta} z^*_\beta$	$\epsilon_{\alpha\beta} z^*_\beta$	z_α	z_α	$\epsilon_{\alpha\beta} z^*_\beta$
u_x	u^*_x	u^*_x	u_y	$-u_x$	u^*_x
u_y	u^*_y	u^*_y	$-u_x$	u_y	u^*_y
v_x	$-v_x$	v_x	v_y	$-v_x$	v_x
v_y	v_y	$-v_y$	$-v_x$	v_y	v_y
v	$-iv^*$	iv^*	iv	$-v^*$	v^*
$f_x = u_x v_x$	$-f^*_x$	f^*_x	f_y	f_x	f^*_x
$g_x = u_x v_y$	$-g^*_x$	g^*_x	g_y	$-g_x$	g^*_x

TABLE I. Symmetry transformations of fields in the compact CP(1) model. Different columns represent actions of corresponding symmetry operations. T_x and T_y: translations by one lattice spacing along x and y directions, respectively; $R_{\pi/2}$: 90-degree rotation about a lattice site; I_x: reflection about the axis of $x = 0$; $\mathcal{T}$: time-reversal operation. z_α are the spinon fields in the CP(1) model in Eq. (1), and its symmetry transformations are summarized in Ref. 26; $u_{x,y}$ are the spinon pair operators defined in Eq. (6); v, v_x, and v_y are skyrmion and VBS order parameters[13] defined in Eq. (5). f_x and g_x are two nematic bound-state operators defined in Eq. (8), and $f_y = u_y v_y$, $g_y = -u_y v_x$ are corresponding operators obtained after rotation.

Our aim is to find a bilinear form of u and v fields that is invariant [up to a U(1) gauge transformation] under all symmetry operations. However, this cannot be achieved, as $R_{\pi/2}$ and T_x do not commute. In other words, condensing a bound state of skyrmion/antiskyrmion and spinon pair will break either the reflectional symmetry or the rotational symmetry. It is more natural that we choose to break the rotational symmetry, as breaking the translation enlarges the unit cell and allows the possibility of a trivial paramagnetic ground state[27]. In the rest of the paper we will consider only Z_2 spin liquid states where the C_4 rotational symmetry of the square lattice is broken down to C_2. In other words, the spin liquid states we obtain in this paper are nematic spin liquid states. The possibility of obtaining a nematic Z_2 spin liquid state in the J_1-J_2 model on a square lattice will be discussed in more details in Sec V.

Finally, we fix the form of bound-state operator by considering the requirement of reflection symmetry. The square lattice has reflection symmetries with respect to both the x and y axes, and the diagonal direction of $x \pm y$. When the four-fold rotation symmetry is broken, only one set of reflection symmetries can be preserved. Here we consider states with reflection symmetries about the x and y axes, since these states have the same lattice symmetry as the $(0, \pi)$ Néel state at large J_2/J_1[10,11]. According to Table I, the reflection symmetry changes v to its complex conjugate, so it turns a skyrmion into an antiskyrmion. Therefore, to have a reflection symmetric condensate, the order parameter needs to be a linear combination of spinon pair– skyrmion bound state and spinon pair–antiskyrmion bound state. We can show that there are two possibilities that satisfy all the symmetries except rotation:

$$f_x = u_x v_x, g_x = u_y v_x. \tag{8}$$

The symmetry transformations of these two fields are also summarized in Table I. Under all symmetry transformations except $R_{\pi/2}$, the two bound-state operators either are invariant or become their complex conjugates, and they may also acquire a minus sign. Using the U(1) gauge invariance, the phase of the bound-state condensate can be fixed to be real, and the extra minus sign can also be canceled by a U(1) gauge transformation. Therefore the states obtained by condensing either f_x or g_x are nematic spin liquid states that preserve all other symmetries listed in Table I.

II. PHASE TRANSITION TO Z_2 SPIN LIQUID STATE.

In this section we discuss the phase transition to the Z_2 spin liquid state and the low-energy excitations in the spin liquid state. We will show that the Z_2 spin liquid state can be reached from the deconfined quantum criticality by proliferating the spinon pair–skyrmion/antiskyrmion bound states. Moreover, the vortex excitations of the bound-state condensate become the vison excitations in the Z_2 spin liquid state.

In the theory of the deconfined quantum criticality, killing the Néel order in a spin-$\frac{1}{2}$ system on square lattice brings the system to the deconfined quantum critical point, which is described by the noncompact CP(1) model. Away from the critical point, the four-skyrmion tunneling events become a dangerously irrelevant perturbation that drives the system into a VBS phase. This phase transition can be described by the following effective Lagrangian:

$$\mathcal{L} = \frac{1}{g}\sum_{\alpha} |(\partial_\mu - ia_\mu)z_\alpha|^2 + \lambda_v \left(v^4 + v^{\dagger 4}\right), \tag{9}$$

where the λ_v term represents four-skyrmion tunneling events.

Similarly, one can go from the deconfined quantum critical point to the Z_2 spin liquid phase with the bound-state operator as another dangerously irrelevant perturbation. Without losing generality, we consider condensing f_x as an example. The operator f_x can be decomposed into two fields describing bound states of spinon pair plus skyrmion or antiskyrmion, respectively:

$$f_x = \frac{1}{2}(f_x^+ + f_x^-), \quad f_x^+ = e^{-i\frac{\pi}{4}} v^\dagger u_x, \quad f_x^- = e^{i\frac{\pi}{4}} v u_x. \tag{10}$$

As bound states, the gauge charge and flux carried by $f_x^\pm$ are the sum of gauge charges carried by the spinon pair and the sum of gauge flux carried by the skyrmion (or antiskyrmion). Hence $f_x^\pm$ carries gauge charge $2e$ and gauge flux $\pm 2\pi$. In the CP(1) model, the gauge charge is conserved, while the flux is conserved modular 8π, as skyrmion number is conserved modular four. Therefore using the symmetry transformations listed in Table I we see that the following Lagrangian with a quartic term of bound-state operator is allowed by all lattice symmetries and gauge charge and flux conservations,

$$\mathcal{L} = \frac{1}{g}\sum_{\alpha} |(\partial_\mu - ia_\mu)z_\alpha|^2 + \lambda_f (f_x^{+2} f_x^{-*2} + \text{H.c.}). \tag{11}$$

At the deconfined quantum critical point, the $f_x^\pm$ fields are gapless as both spinon pair and skyrmion/antiskyrmion fields are gapless. When we move away from the critical point, the λ_f term in Eq. (11) becomes relevant and leads to the bound-state condensation. To be precise, this quartic term pins the phases of $f_x^\pm$ fields, which breaks the U(1) gauge symmetry in the CP(1) down to Z_2 and breaks the fourfold rotational symmetry. We leave the study of the renormalization group flow of this new quartic term to future works and only assume that such a scenario of deconfined criticality is possible. In the rest of this section we discuss the low-energy excitations in the phase obtained through bound-state condensation and argue that it is a gapped spin liquid state with Z_2 topological order.

Excitation	Gauge charge	Gauge flux
z_α	e	0
v	0	2π
$f_x^\pm$	$2e$	$\mp 2\pi$
Vortex of $f_x^\pm$	$\mp e/2$	$\pi/2$

TABLE II. Gauge charge and gauge flux assignments of low-energy excitations. In the table z_α is spinon excitations in the CP(1) model, v is skyrmion excitation, and $f_x\pm$ is the bound state of spinon pair and antiskyrmion/skyrmion defined in Eq. (10).

As we are condensing the bound state of spinon pair and skyrmion, the spinon excitations remain well defined in the condensed phase. Since the condensate carries gauge flux $\pm 2\pi$, the spinons are gapped. Therefore in the condensed phase there are spin-$\frac{1}{2}$ spinons carrying gauge charge e. On the other hand, in the condensed phase there are also vortex excitations of the bound-state condensate. Near the aforementioned critical point we have two condensates of $f_x^\pm$, because the relative phase of the two is allowed to fluctuate due to the irrelevance of the fourfold rotational lattice anisotropy at the deconfined quantum critical point. Consequently, there exist two types of topological excitations that are 2π vertices of the two condensates. The gauge charge and flux carried by these excitations can be worked out by considering the mutual statistics between the bound-state operators and their vortices: there is a 2π Berry phase if we move an $f_x^\pm$ bound state quasiparticle around the corresponding vortex, and there is no Berry phase if we move an $f_x^\pm$ bound state around the vortex of the opposite condensate $f_x^\mp$. Using this condition and the gauge charge/flux assignment of $f_x^\pm$, we can derive the following gauge charge/flux assignment of the vortices: the vortex of f_x^+ carries gauge charge $-e/2$ and gauge flux $\pi/2$, and the vortex of f_x^- carries carries gauge charge $e/2$ and gauge flux $\pi/2$. These results are listed in Table II. Near the critical point there are vortex excitations of $f_x^\pm$ carrying fractionalized gauge charge and flux. However, when we move away from the critical point into the bound state condensed phase, the phases of $f_x^\pm$ are locked by the quartic term in Eq. (11) and there is only one condensate of the linear combination of $f_x^\pm$ as shown in Eq. (10). Therefore the vortices of $f_x^\pm$ are confined together and the bound state of two $f_x^\pm$ vortices carries no gauge charge and gauge flux of π. In conclusion, in the bound state condensed phase there are two types of low-energy excitations: spinons carrying gauge charge e and bound state of $f_x^{\pm}$ vortices carrying gauge flux π, and they see each other as π flux. Therefore these two types of excitations can be treated as spinon and vison excitations in a Z_2 spin liquid state, and consequently the phase we get by condensing a spinon pair–skyrmion/antiskyrmion bound state is a gapped spin liquid state with Z_2 topological order.

Moreover, from this analysis one can see that both spinon and vison gaps close at the critical point: The spinon gap closes since the spinon condenses to form the Néel order as we go across the critical point; the vison gap closes because the vortex core energy vanishes as the stiffness of the $f_x^{\pm}$ condensates vanishes at the critical point. This is consistent with the findings in the numerical studies[10,11] that the gaps of spin-singlet and spin-triplet excitations close as one approaches the quantum critical point from the spin liquid side, and that both spin-spin and dimer-dimer correlations have power-law behavior at the critical point.

III. SCHWINGER BOSON MEAN FIELD STATE.

In this section we construct a microscopic description of the nematic spin liquid state obtained by condensing bound-state operator using the Schwinger boson representation. The Schwinger boson method has been used to study different spin models. Particularly, the nearest neighbor Heisenberg model on square lattice has been studied using a U(1) Schwinger boson spin liquid theory[19,20]. Models with frustrations, like the J_1-J_2 model, can be studied using a Z_2 Schwinger boson spin liquid theory[9]. In both cases, the Schwinger boson representation introduces fractionalized spinons and emergent gauge fields. Therefore, different projective ground state wave functions have different topological orders which can be classified using their PSG. Here we construct the particular mean field Hamiltonian that gives the projective ground state corresponding to the spin liquid which we obtain by the effective theory, by matching the PSG of the mean field Hamiltonian to the PSG obtained in Table I.

In the Schwinger boson representation, the spin degree of freedom is expressed using two flavors of bosons carrying spin-$\frac{1}{2}$,

$$\boldsymbol{S}_i = a_{i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} a_{i\beta}, \tag{12}$$

where $\boldsymbol{\sigma}$ is a vector formed by the three Pauli matrices, α, β are spin indices taking values of up and down, and $a_{i\alpha}$ are Schwinger boson operators carrying spin-$\frac{1}{2}$. To relate the Schwinger boson representation to the CP(1) model discussed in Sec. I, we adapt the notation in Ref. 7 where the Schwinger boson operator is redefined on sublattice B as the following,

$$b_{i\alpha} = \begin{cases} a_{i\alpha}, & i \in A, \\ \epsilon_{\alpha\beta} a^\dagger_{i\beta}, & i \in B, \end{cases} \tag{13}$$

where $\epsilon_{\alpha\beta}$ is the total antisymmetric tensor. After this canonical transformation, the operator $b_{i\alpha}$ is related to the physical spin operator as $(-1)^i \boldsymbol{S}_i = b^\dagger_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} b_{i\beta}$, which has a similar form as Eq. (2). Hence one can view the CP(1) field z_α as the long-wavelength mode of $b_{i\alpha}$.

We start with a U(1) spin liquid state that corresponds to the deconfined quantum critical point described by the CP(1) model. Such state can be given by the following mean field Hamiltonian that contains a uniform hopping term on nearest-neighbor bonds[28],

$$H^{\mathrm{nn}}_{\mathrm{MF}} = -P \sum_{\langle ij \rangle} \left(b^\dagger_{i\alpha} b_{j\alpha} + \mathrm{H.c.} \right), \tag{14}$$

where P is a mean field order parameter representing the hopping matrix element on nearest-neighbor bonds. This mean field Hamiltonian is invariant under U(1) gauge transformation $b_{i\alpha} \to b_{i\alpha} e^{i\theta}$, and hence it is coupled to an emergent U(1) gauge field. Moreover, the symmetry transformation of the spinon operator $b_{i\alpha}$, as summarized in Table III, is the same as the CP(1) spinon field z_α[26]. Consequently the U(1) spin liquid state described here using Schwinger bosons represents the same deconfined quantum critical point as in the case of the CP(1) model in Eq. (1), and the low-energy mode of $b_{i\alpha}$ corresponds to z_α.

	T_x	T_y	$R_{\pi/2}$	I_x	$\mathcal{T}$
$b_{i\alpha}$	$\epsilon_{\alpha\beta} b^*_{j\beta}$	$\epsilon_{\alpha\beta} b^*_{j\beta}$	$b_{j\alpha}$	$b_{j\alpha}$	$\epsilon_{\alpha\beta} b^*_{j\beta}$

TABLE III. Symmetry transformations of spinon in Schwinger boson mean field state[26].

Next, we study Z_2 spin liquid states adjacent to the deconfined quantum critical point. Naturally, such states can be constructed on top of this U(1) spin liquid state. Motivated by the J_1-J_2 model, we consider adding the following pairing term on the diagonal bonds, which can lower the mean-field energy due to the J_2 coupling in the Hamiltonian,

$$H^{\mathrm{nnn}}_{\mathrm{MF}} = \sum_{\langle\langle ij \rangle\rangle} \left(Q^*_{ij} \epsilon_{\alpha\beta} b_{i\alpha} b_{j\beta} + Q_{ij} \epsilon_{\alpha\beta} b^\dagger_{i\alpha} b^\dagger_{j\beta} \right), \tag{15}$$

where Q_{ij} is the mean-field order parameter representing pairing on next-nearest-neighbor (or diagonal) bonds, and it is proportional to the mean-field expectation value of the spinon pair operator,

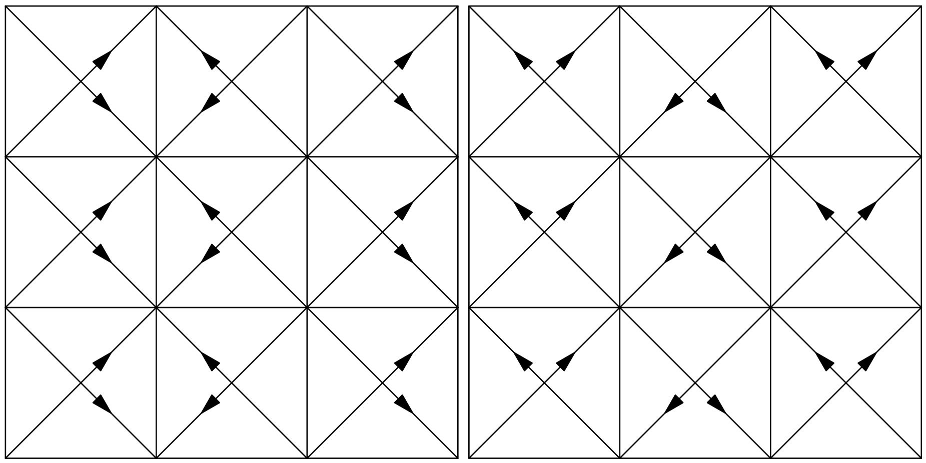
$$Q_{ij} \propto \langle \hat{A}_{ij} \rangle, \quad \hat{A}_{ij} = \epsilon_{\alpha\beta} b_{i\alpha} b_{j\beta}. \tag{16}$$

Such a pairing term breaks the U(1) gauge symmetry and therefore changes the gauge fluctuation to Z_2 through the Higgs mechanism.

In Sec. I, the Z_2 spin liquid state is obtained by condensing the bound-state operator defined in Eq. (8). In analogy, the Z_2 spin liquid state described here using Schwinger boson framework is obtained by condensing pairs of Schwinger boson operators. Consequently, in order to realize the same Z_2 spin liquid state using Schwinger bosons, we need to find the particular form of the spinon pair operator that corresponds to the bound-state operator. At first glance, this task is not trivial because the bound-state operator carries a skyrmion quantum number, which is a topological defect of the spin state. In the theory of the deconfined quantum criticality, the skyrmion operator is related to the order parameter of the VBS state using the argument that the two operators transform in the same way under all symmetry transformations, and therefore have the same scaling behavior near the critical point[13]. Similarly, we can find the form of the bound-state operator in terms of Schwinger boson operators by comparing how they transform under symmetry operations. In our case, we need to find a Schwinger boson pair operator that has not only the same symmetry, but also the same PSG as the bound-state operator, as both operators carry gauge charge $2e$ and are thus gauge covariant. Moreover, having the same PSG suggests that the two states have the same topological order, which is required if they are indeed the same state.

The symmetry and topological order of the Z_2 spin liquid ground state specified by the mean-field Hamiltonian in Eqs. (14) and (15) are determined from analyzing the PSG of the mean-field order parameters, particularly the diagonal pairing order parameter Q_{ij}. Lattice symmetries and time-reversal symmetry require that Q_{ij} takes real values with the same absolute value on all bonds, but it can have different signs on different bonds. The sign of Q_{ij} can be conveniently expressed by specifying an orientation of the bond along which Q_{ij} is positive, as $Q_{ij} = -Q_{ji}$. Hence a pattern of Q_{ij} can be determined by specifying orientations of all diagonal bonds. Then the PSG of this pattern can be worked out using the signs of Q_{ij} and the symmetry transformation of Schwinger boson operators listed in Table III. By matching the symmetry transformation with the PSG of the bound-state operator listed in

Table I, we find the configuration of Q_{ij} that gives the same spin liquid state as obtained in Sec. I by condensing f_x and g_x operators, and the configurations we find are plotted in Fig. 2.



(a)f_x (b)g_x

FIG. 2. Pattern of pairing order parameters Q_{ij} in Eq. (15). The arrows show the direction along which Q_{ij} is positive. The two patterns correspond to spin liquid states obtained by condensing f_x and g_x as defined in Eq. (8), respectively.

IV. VARIATIONAL MONTE CARLO STUDY.

In this section we study the ground-state wave function of the Schwinger boson projective ansatz using the variational Monte Carlo (VMC) method. Here our primary goal is to illustrate that the projective ansatz we propose based on the effective theory analysis has a relatively low variational energy and is a possible candidate state. Due to the sign problem in the VMC simulation, our study cannot determine whether the Schwinger boson projective ansatz is the ground state of the J_1-J_2 model.

Applying a Gutzwiller projection on mean-field ground-state wave functions is a commonly used technique to improve the mean-field results[29], and such a projection can be evaluated using the VMC method. While being a popular technique to study fermionic projective ansatzes, the VMC method is hard to apply to Schwinger boson wave functions due to the difficulty of calculating permanents[30].

Here we use an alternative VMC method that is based on the non-orthogonal valence bond basis, which is first introduced by Liang *et al.*[24]. The Schwinger boson mean-field ground-state wave function can be easily written in the valence bond basis. Following the notation in Ref. 31, the wave function has the following form:

$$|\Psi\rangle = \sum_{V_r} w(V_r)|V_r\rangle, \tag{17}$$

where V_r denotes different spin-singlet valence bond covering configurations,

$$|V_r\rangle = |(a_1^r, b_1^r), (a_2^r, b_2^r), \dots (a_{N/2}^r, b_{N/2}^r)\rangle, \tag{18}$$

with a_i^r and b_i^r denoting the lattice sites of the ith valence bond, and we assume that the weight of each configuration is given by a product of the weight of each bond,

$$w(V_r) = \prod_i w(a_i^r, b_i^r). \tag{19}$$

Using the $a_{i\alpha}$ Schwinger boson operators, the mean field Hamiltonian in Eq. (14) and (15) has the following form,

$$H_{\mathrm{MF}} = -\sum_{\langle ij\rangle} P_{ij}\left(a_{i\alpha}^\dagger a_{j\alpha} + \mathrm{H.c.}\right) + \sum_{\langle\langle ij\rangle\rangle}\left(Q_{ij}^*\epsilon_{\alpha\beta}a_{i\alpha\beta} + \mathrm{H.c.}\right), \tag{20}$$

and contains pairing terms on both nearest-neighbor and diagonal bonds. As a result, after applying the Gutzwiller projection, the Schwinger boson mean-field wave function can be written in forms of Eq. (17) with weights $w(V_r)$ determined from the mean-field Hamiltonian[30]. However, here we use a more general form of variational wave function where we assume that the absolute value of the weights depends only on the Manhattan distance of the bond and use weights of different bonds instead of the parameters in the mean-field Hamiltonian as variational parameters.

On the other hand, the sign of the weights is determined from the projective symmetry group of the mean-field ansatz. For a U(1) spin liquid ansatz, the ground state in Eq. (20) contains only valence bond pairings between two sublattices and the weights are all positive(the orientation of bonds is chosen to be pointing from sublattice A to sublattice B[24]). Therefore the VMC does not have any sign problem and converges rapidly. However, the Z_2 spin liquid state obtained after condensing the spinon pair operator in Eq. (16) does create the sign problem in the VMC calculation. However, for a finite size the sign problem can be overcome by brutal force if the diagonal pairing amplitude is small enough.

We perform the VMC calculation using the improved loop update algorithm[31]. To study the U(1) spin liquid state, we go beyond a simple mean-field ansatz of Eq. (20) and allow pairings on all inter-sublattice bonds. We assume that the weights of bonds depends only on the Manhattan length of the bonds and use the weights as variational parameters. On a 32-by-32 sites system we obtain a ground state energy of $-0.4893(2)J_1$ per site with $J_2 = 0.5J_1$, and $-0.4748(2)J_1$ with $J_2 = 0.55J_1$. Comparing to the ground state energy of $-0.4943J_1$ for $J_2 = 0.5J_1$ and $-0.4844J_1$ for $J_2 = 0.55J_1$ obtained in Ref. 11, this suggests that a bosonic U(1) spin liquid state is a reasonable starting point in understanding the spin liquid phase in the J_1-J_2 model. The bond weights $w(a, b)$ obtained from the variational calculation decay exponentially as the length of the bond increases, indicating that the spin liquid state has short-range spin-spin correlation[24]. Here we emphasize that this wave function corresponds to the parent critical U(1) state described by the critical CP(1) model or the U(1) Schwinger boson ansatz, not the gapped Z_2 spin liquid state, which we will discuss briefly later (hence we do not expect this wave function to give a low variational energy as compared to other numerical methods). Particularly, this wave function contains only short-ranged intersublattice bonds and therefore has a U(1) topological order. As a result, it has a critical dimer-dimer correlation[32].

Starting from this critical U(1) spin liquid state, we obtain a Z_2 spin liquid state by adding a small weight of diagonal pairing, and the signs of the diagonal pairing are given by the ansatz shown in Fig. 2. The numerical results are listed in Table IV. For either ansatz, we observe that there is no change in the ground-state energy within our statistical errors, but for the f_x ansatz, introducing the diagonal pairing creates anisotropy in nearest-neighbor spin-spin correlation. In other words, the Z_2 spin liquid state with a diagonal pairing does not improve the energy. Our numerical study suggests that the bosonic nematic spin liquid state has a low ground-state energy as a variational state, but whether it is the ground state of the J_1-J_2 model cannot be concluded from our variational calculation. On the other hand, the anisotropic $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$ on nearest-neighbor bonds implies that this nematic spin liquid state has a lower energy in an anisotropic J_{1x}-J_{1y}-J_2 model, where the nearest-neighbor antiferromagnetic interactions in the x and y directions are different: $J_{1x} \neq J_{1y}$. There have been numerical studies on this J_{1x}-J_{1y}-J_2 model[33] that show the existence of an intermediate nonmagnetic phase between the Néel state and another antiferromagnetic phase with a $(\pi, 0)$ order for a finite range of J_{1x}/J_{1y} around 1. This suggests that such a spin liquid phase also exists when $J_{1x} \neq J_{1y}$, and the nematic Schwinger boson projective wave function we study in this work may describe such a spin liquid state in the anisotropy J_{1x}-J_{1y}-J_2 model.

Wave function	Energy per site/J_1	$\lvert(C_x - C_y)/(C_x + C_y)\rvert$
$w_d = 0$	$-0.489281(1)$	0
f_x, $w_d = 0.005$	$-0.489280(1)$	0.000045(10)
f_x, $w_d = 0.01$	$-0.489284(3)$	0.000184(26)
g_x, $w_d = 0.005$	$-0.489282(1)$	0.000017(10)
g_x, $w_d = 0.01$	$-0.489281(3)$	0.000023(26)

TABLE IV. Energy and anisotropy of nearest neighbor spin-spin correlation of variational wave functions. In the first column, w_d denotes the weight of the diagonal bonds defined in Eq. (19), relative to the weight of nearest-neighbor bonds. f_x and g_x, respectively, denote the pattern shown in the two subfigures in Fig. 2. The second column shows the energy per site in units of J_1, and the third column shows the anisotropy of nearest-neighbor spin-spin correlations, where $C_{x,y} = \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+x,y} \rangle$ is the nearest-neighbor spin-spin correlation in x and y directions, respectively. The number in the parenthesis shows the standard error. Note that the energies listed here have smaller errors compared to the ground-state energy $-0.4893(2)$ given in the main text, because the errors listed here contain only the statistical errors in the Monte Carlo simulations, whereas the main error in the ground-state energy data provided in the main content comes from minimizing the energy of trial wave function.

V. CONCLUSIONS

In this paper we have discussed a possible scenario of obtaining a Z_2 spin liquid phase from the Néel phase in a spin-$\frac{1}{2}$ system on a square lattice through a continuous phase transition by condensing a bound state of spinon pair and skyrmion excitations. The symmetry of the spin liquid state is studied using PSG analysis. While condensing the skyrmion itself breaks the translational symmetry, the bound-state condensation does not break this symmetry and leads to a translational symmetric spin liquid state. Near the critical point, the vortices of the condensate carry fractionalized gauge charge and flux, but they are confined in the spin liquid phase and are combined to form vison excitations in the Z_2 gauge theory. Moreover, we can describe the Z_2 spin liquid state using a Schwinger boson projective wave function and the bound-state operator maps to a pairing operator on diagonal bonds with a certain PSG. We calculate the ground-state energy of the Schwinger boson projective wave function using the variational Monte Carlo method and find that it has a relatively low energy. The spin liquid state we obtain has the Z_2 topological order, and therefore the entanglement entropy contains the universal constant $\gamma = \ln 2$, which is consistent with the observations in numerical studies[10,11].

The spin liquid state we obtain in this work is nematic as it has all translational symmetries of the square lattice but breaks the fourfold rotational symmetry down to twofold. The result that we could not find a rotational symmetric spin liquid state is consistent with previous studies on slave-particle constructions of spin liquid states on the square lattice. On one hand, using the Schwinger boson framework, nematic spin liquid states have been proposed on a square lattice[7,8], and have been used to study the J_1-J_2 model[9]. Moreover, the PSG analysis[34] shows that all bosonic spin liquid states that have zero-flux hopping on nearest-neighbor bonds and nonvanishing pairing on diagonal bonds are nematic. In other words, all Z_2 spin liquid states obtained by adding pairing on diagonal bonds on top of the U(1) spin liquid state are nematic. On the other hand, the PSG analysis on fermionic spin liquid states[22] shows that there is no rotational symmetric gapped Z_2 spin liquid state adjacent to the π-flux U(1) spin liquid state. In summary, neither a bosonic nor fermionic slave particle framework can describe a rotational symmetric gapped Z_2 spin liquid state that can be connected to the Néel state through a continuous phase transition. Furthermore, we note that a similar lattice symmetry-breaking spin liquid state is proposed for the kagome lattice Heisenberg model[35]. However, on the square lattice the lattice symmetry breaking plays a more crucial role in the Z_2 spin liquid state, because without such symmetry breaking the spin liquid state would be coupled to a U(1) gauge field instead, which would make it unstable in two dimensions[28].

One key result of this theoretical work is that on the square lattice, the gapped spin liquid state obtained through a direct second-order phase transition from the Néel state is a nematic spin liquid state that breaks the four-fold rotational symmetry. Such symmetry breaking is neither observed nor ruled out in numerical studies of the J_1-J_2 model. On one hand, the system studied in Ref. 10 using the density matrix renormalization group (DMRG) method is a ladder system and does not have the rotational symmetry to begin with. On the other hand, in the work of Wang *et al.*[11] rotational symmetry of the ground state was not explicitly checked. We hope the rotational symmetry of the spin liquid state can be clarified by future numerical studies. Moreover, recent numerical studies using DMRG[36] and VMC methods[37] provide evidence for a gapless spin liquid state. Therefore we hope future numerical studies can resolve this controversy and determine whether our critical theory can be applied to the J_1-J_2 model on a square lattice.

Even though the nematic spin liquid state we have proposed may not describe the ground state of the J_1-J_2 model, it still might be realized in a model that lacks C_4 lattice rotational symmetry, as suggested by our variational study described in Sec. IV. We note that our theoretical analysis in Sec. I–III also applies to an anisotropic model. Particularly, the symmetry transformations listed in Table I generate all lattice symmetry operations of an anisotropic square lattice if one replaces the rotation $R_{\pi/2}$ by $R_\pi = R_{\pi/2}^2$. Hence the same novel quantum critical point between the Néel and the Z_2 spin liquid state also exists in an anisotropic model. Therefore it will be interesting to study the anisotropic J_{1x}-J_{1y}-J_2 model to see if the anisotropy helps to stabilize the nematic spin liquid state found in this work.

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